Algebraic Multigrid Techniques for the eXtended Finite Element Method

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Thanks to: E. Boman, J. Gaidamour (Sandia),
B. Hiriyur, H. Waisman (Columbia U.)

- Motivation
  - A brief review of XFEM & Smoothed Aggregation - Algebraic Multigrid (SA-AMG)
    - Why does standard SA-AMG fail & how to fix it
      - Examples
        - Conclusion

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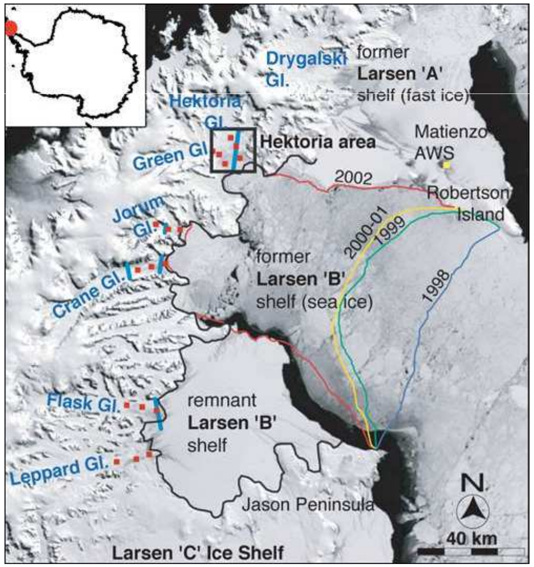
Fracture of ice

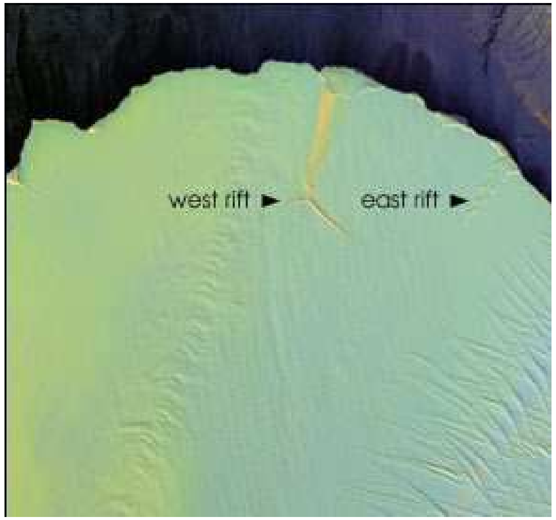
Objective: Employ parallel computers to better understand how fracture of land ice affects the global climate. Fracture happens e.g. during

- the collapse of ice shelves,
- the calving of large icebergs, and
- the role of fracture in the delivery of water to the bed of ice sheets.

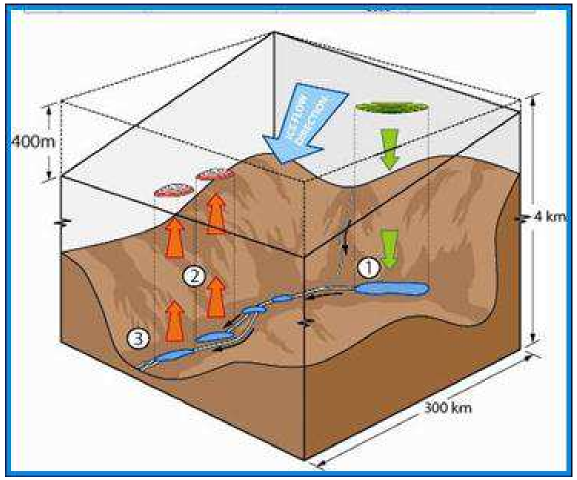
Ice shelves in Antarctica:



Larsen ‘B’ diminishing shelf 1998-2002
Other example: Wilkins ice shelf 2008



Amery ice shelf

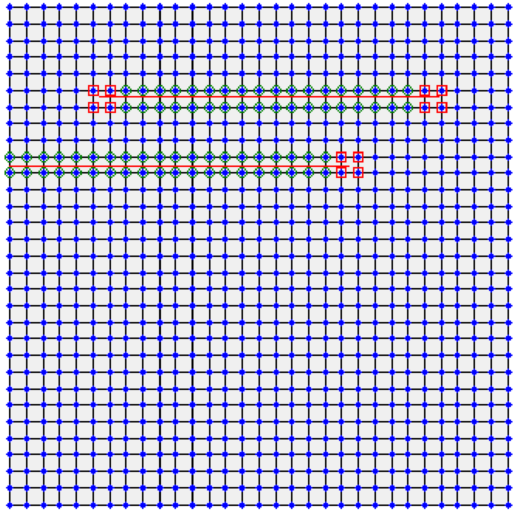


Glacial hydrology
(Source: http://www.sale.scar.org)

Linear elastic XFEM Formulation for Cracks

Displacement approximation (shifted basis form.)

$$
\begin{aligned}
u^h(\mathrm{x}) \quad = \quad & \sum_{I=1}^{n} N_I(\mathrm{x}) u_I \\
& + \sum_{i=1}^{n_h} N_{I_i}(\mathrm{x}) \left(H(\mathrm{x}) - H\left(\mathrm{x}_{I_i}\right)\right) a_{I_i} \\
& + \sum_{i=1}^{n_f} N_{\hat{I}_i}(\mathrm{x}) \sum_{J=1}^{n_J} \left(F_J(\mathrm{x}) - F_J\left(\mathrm{x}_{\hat{I}_i}\right)\right) b_{\hat{I}_i J}
\end{aligned}
$$



- Jump Enrichment

$$
H(\boldsymbol{x}) = \begin{cases} 0.5 & \text{in } \Omega^+ \\ -0.5 & \text{in } \Omega^- \end{cases}
$$

- Tip Enrichment (brittle crack)

$$
F_J(r,\theta) = \left\{ \overbrace{\sqrt{r}\sin\left(\frac{\theta}{2}\right)}^{J=1}, \overbrace{\sqrt{r}\cos\left(\frac{\theta}{2}\right)}^{J=2}, \overbrace{\sqrt{r}\sin\left(\frac{\theta}{2}\right)\sin(\theta)}^{J=3}, \overbrace{\sqrt{r}\cos\left(\frac{\theta}{2}\right)\sin(\theta)}^{J=4} \right\}
$$

Bubnov-Galerkin method → Symmetric global system

$$
\boldsymbol{A} = \sum_e \int_{\Omega_e} \boldsymbol{B}_e^{\mathrm{T}} \boldsymbol{C} \boldsymbol{B}_e \, \mathrm{d}\boldsymbol{x}
$$

$$
\boldsymbol{f} = \sum_e \int_{\Gamma_e} \boldsymbol{N}_e^{\mathrm{T}} h \, \mathrm{d}\boldsymbol{x} + \sum_e \int_{\Omega_e} \boldsymbol{N}_e^{\mathrm{T}} \rho \, \mathrm{d}\boldsymbol{x}
$$

$$
\boldsymbol{A}\boldsymbol{u} = \boldsymbol{f}
$$

Current implementation: bi-linear, Lagrange polynomials, quad4 elements

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Multigrid principles

- Oscillatory components of error are reduced effectively by smoothing, but smooth components attenuate slower

  → capture error at multiple resolutions using grid transfer operators $\boldsymbol{R}^{[k]}$ and $\boldsymbol{P}^{[k]}$

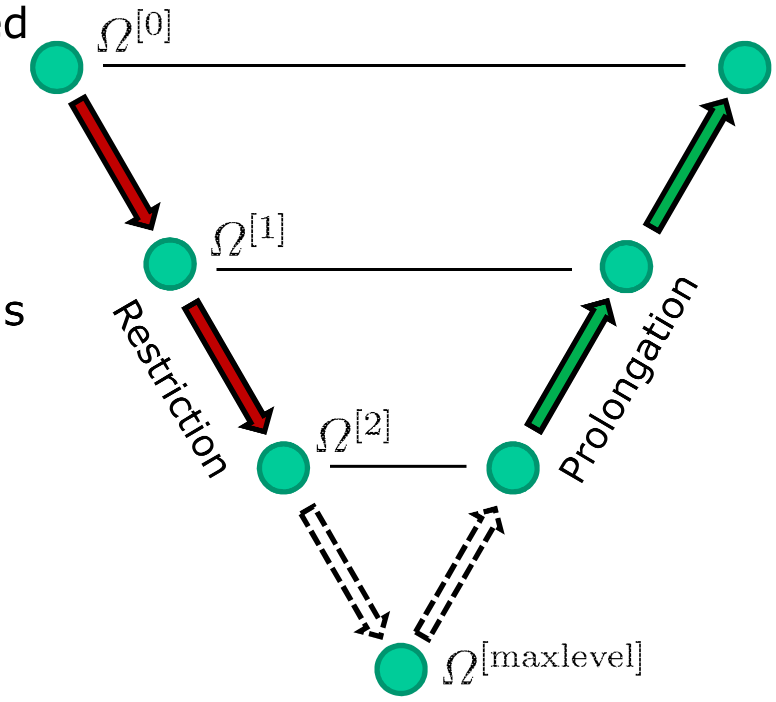
  → optimal number of linear solver iterations

- In **AMG**, transfer operators are obtained from **graph information of *A***

  → ideal for general, unstructured meshes

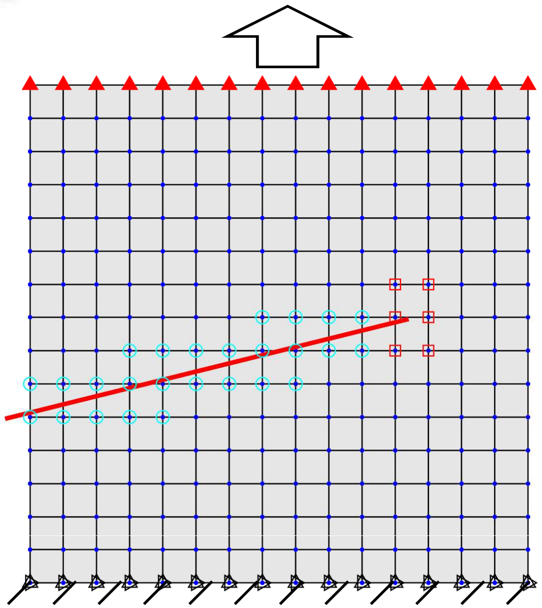
solve Au=b using recursive multilevel V Cycle:

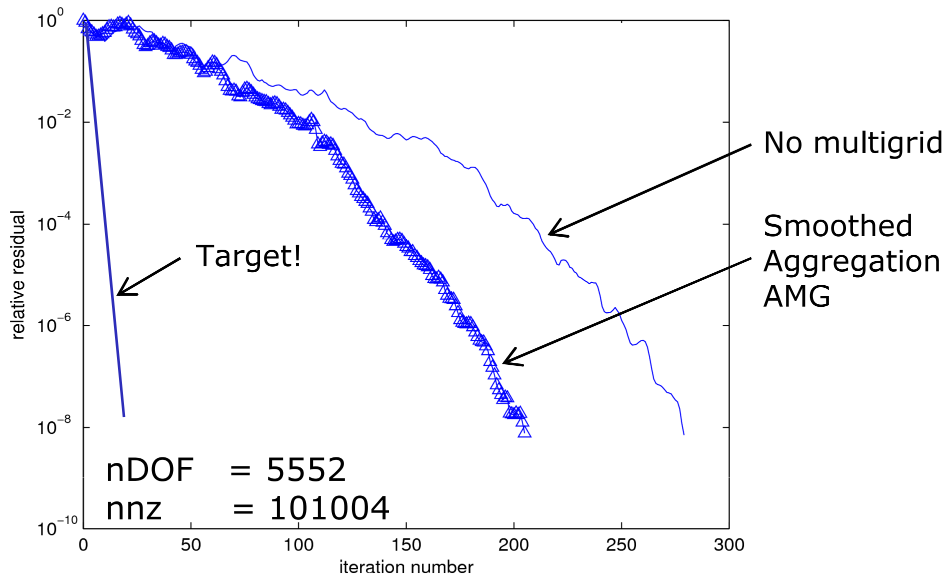
```
function u ← multilevel(b, u, k)
 smooth (pre-smoothing)
 If k < maxlevel:
    restrict u to coarser level
    compute u on coarser level
    interpolate u to finer level
    smooth (post-smoothing)
 return u
```



- iterative smoothers on finest and intermediate levels
- direct solve at the coarsest level

'Standard' SA-AMG for fracture problems

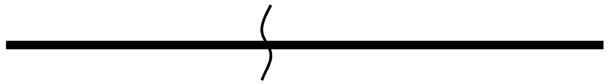




Possible issues:

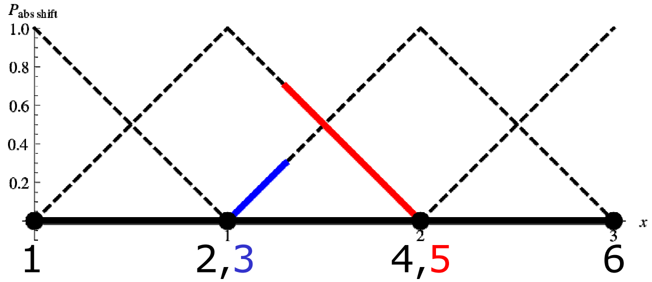
- XFEM matrix graph messes with aggregation
  - Assumption of 2 unknowns per node not true
  - Aggregates should not cross crack
- How to define rigid body modes?
  - Modes are used to define nullspace
- How to deal with large condition numbers?
  - Define smoothers for each level

Distinct region representation



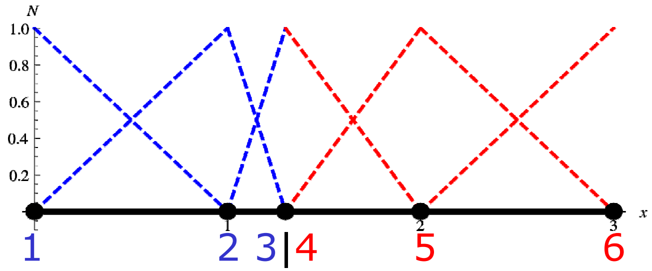
K | M

XFEM: modified shifted enrichment $\sum_I N_I(x)\,|H(x)-H(x_I)|\,a_I$



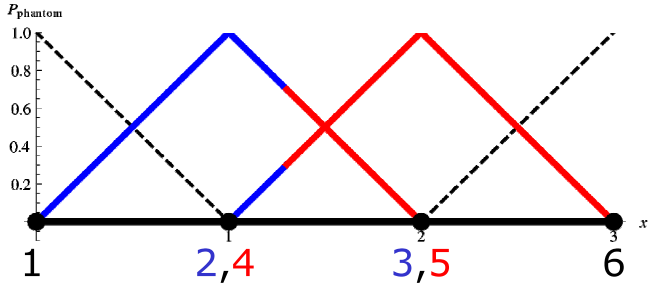
$$\frac{EA}{2h_1}\begin{bmatrix} 2 & -2 & 0 & 0 & 0 & 0 \\ -2 & 4 & 1 & -2 & -1 & 0 \\ 0 & 1 & 1 & -1 & 0 & 0 \\ 0 & -2 & -1 & 4 & 1 & -2 \\ 0 & -1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & -2 & 0 & 2 \end{bmatrix} \qquad \frac{\rho A h_1}{24}\begin{bmatrix} 8 & 4 & 0 & 0 & 0 & 0 \\ 4 & 16 & 1 & 4 & 2 & 0 \\ 0 & 1 & 1 & 2 & 0 & 0 \\ 0 & 4 & 2 & 16 & 1 & 4 \\ 0 & 2 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 4 & 0 & 8 \end{bmatrix}$$

FEM



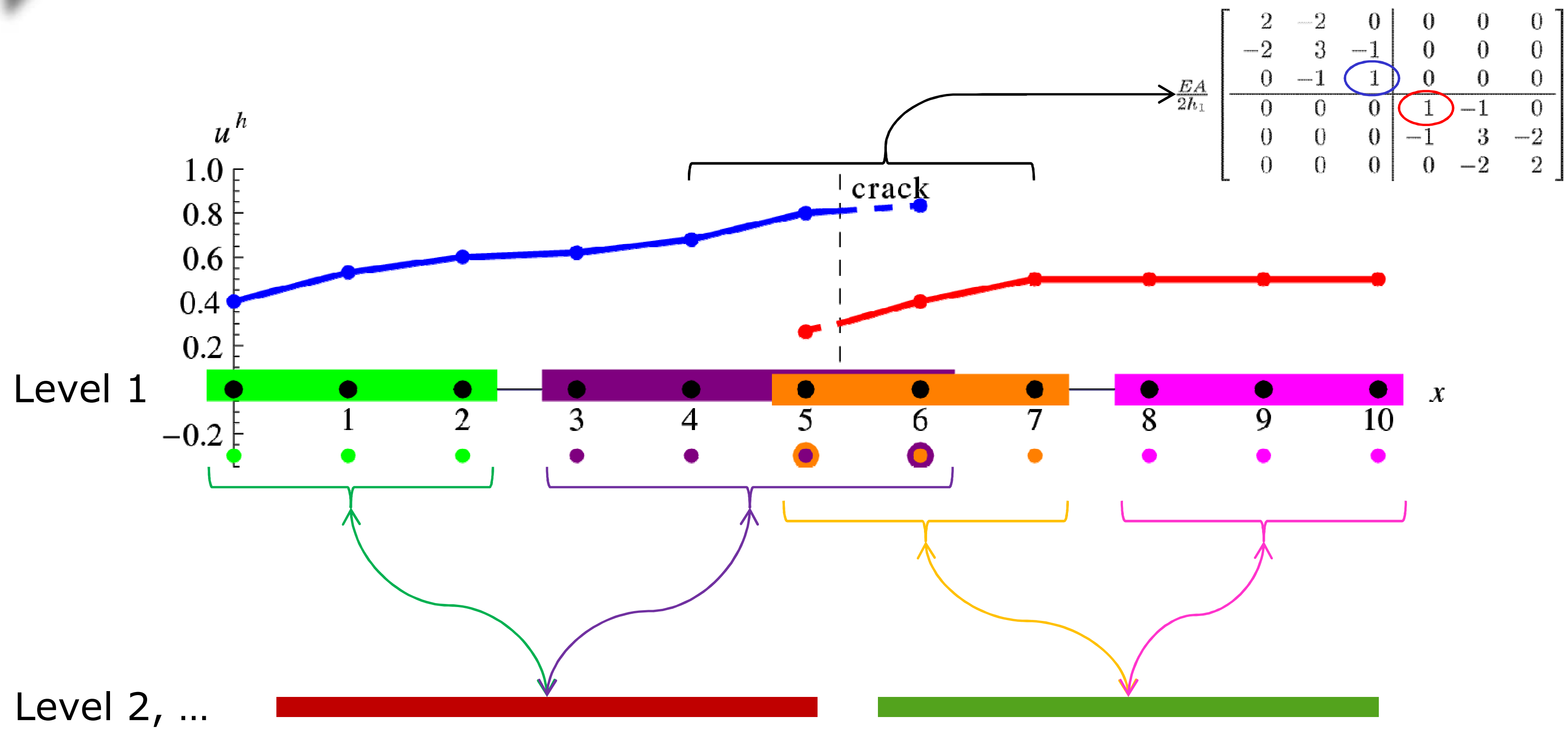
$$\frac{EA}{2h_1}\left[\begin{array}{ccc|ccc} 2 & -2 & 0 & 0 & 0 & 0 \\ -2 & 6 & -4 & 0 & 0 & 0 \\ 0 & -4 & 4 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 4 & -4 & 0 \\ 0 & 0 & 0 & -4 & 6 & -2 \\ 0 & 0 & 0 & 0 & -2 & 2 \end{array}\right] \qquad \frac{\rho A h_1}{24}\left[\begin{array}{ccc|ccc} 8 & 4 & 0 & 0 & 0 & 0 \\ 4 & 12 & 2 & 0 & 0 & 0 \\ 0 & 2 & 4 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 4 & 2 & 0 \\ 0 & 0 & 0 & 2 & 12 & 4 \\ 0 & 0 & 0 & 0 & 4 & 8 \end{array}\right]$$

Phantom node approach



$$\frac{EA}{2h_1}\left[\begin{array}{ccc|ccc} 2 & -2 & 0 & 0 & 0 & 0 \\ -2 & 3 & -1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & -1 & 3 & -2 \\ 0 & 0 & 0 & 0 & -2 & 2 \end{array}\right] \qquad \frac{\rho A h_1}{24}\left[\begin{array}{ccc|ccc} 8 & 4 & 0 & 0 & 0 & 0 \\ 4 & 15 & 2 & 0 & 0 & 0 \\ 0 & 2 & 1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 & 2 & 0 \\ 0 & 0 & 0 & 2 & 15 & 4 \\ 0 & 0 & 0 & 0 & 4 & 8 \end{array}\right]$$

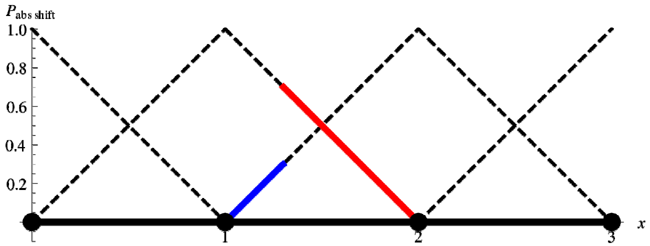
Aggregation for phantom nodes: 1D



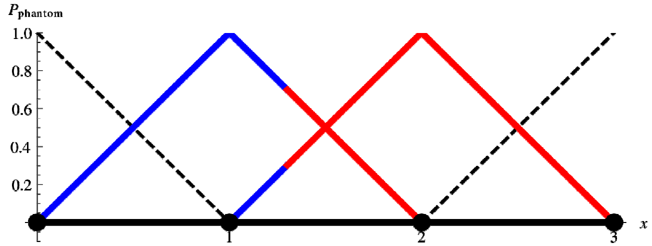
Aggregates are **not** connected on any level!

Change of basis: 1d

Do XFEM developers have to use the phantom node approach? No!



XFEM: modified shifted enrichment



Phantom node approach

For each node I with jump DOFs: $\phi_I - \bar{\phi}_I = \phi_\alpha$

$$\bar{\phi}_I = \bar{\phi}_\alpha$$

$$\boldsymbol{G}^{\mathrm{T}} \cdot \boldsymbol{A} \cdot \boldsymbol{G} \cdot \boldsymbol{G}^{-1} \cdot \boldsymbol{u} = \boldsymbol{G}^{\mathrm{T}} \cdot \boldsymbol{f}$$

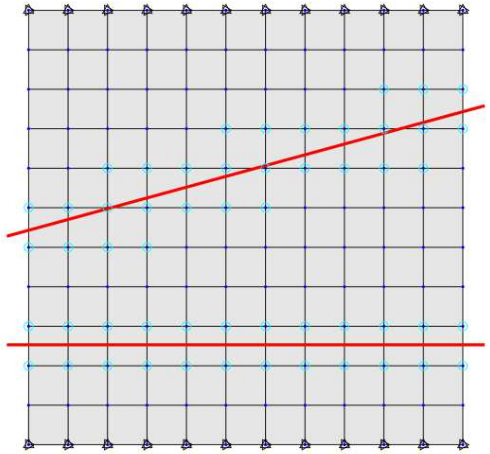
$$\boldsymbol{G}^{\mathrm{T}} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

(similar: Menouillard 2008, …)

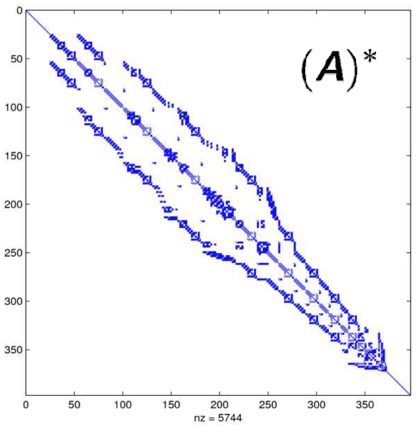
G

- is extremely sparse,
- is simple to produce,
- exists for higher order Lagrange Polynomials and multiple dimensions.

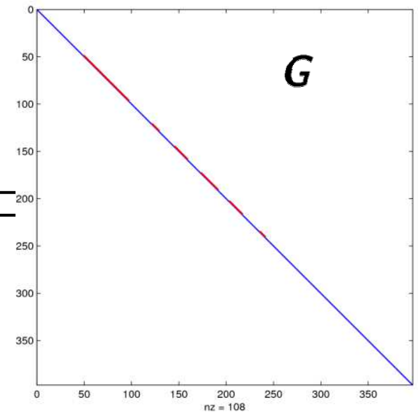
Change of basis: 2d



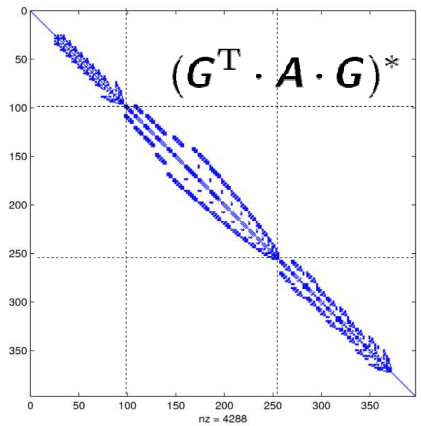
Mesh + BC + Enrichment



Modified shifted enrichment



$$\boldsymbol{G}^{\mathrm{T}} \cdot \boldsymbol{A} \cdot \boldsymbol{G} \cdot \boldsymbol{G}^{-1} \cdot \boldsymbol{u} = \boldsymbol{G}^{\mathrm{T}} \cdot \boldsymbol{f}$$



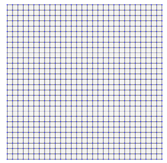
Phantom node approach

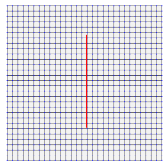
( )* → sym. rev. Cuthill-McKee permutation for visualization

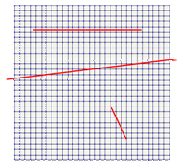
Prelim. results for jump enrichments only

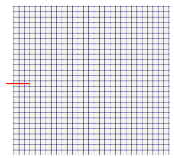
Conj. Gradient preconditioned with AMG

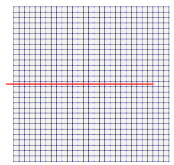
A	Shifted enrichment
$G^{\mathrm{T}} \cdot A \cdot G$	Phantom node











Case	$n_e \times n_e$	$\alpha_{\text{cond.}}$	n_{iter} A 1L	n_{iter} A ML	n_{iter} $G^{\mathrm{T}} \cdot A \cdot G$ 1L	n_{iter} $G^{\mathrm{T}} \cdot A \cdot G$ ML
I	30×30	3e+03	32	9	32	9
	60×60	1e+04	63	10	63	10
	90×90	3e+04	93	11	93	11
	120×120	5e+04	123	11	123	11
II	30×30	2e+06	59	40	53	12
	60×60	1e+06	109	58	104	13
	90×90	2e+06	159	65	156	14
	120×120	1e+07	-	81	-	15
III	30×30	1e+04	46	25	42	11
	60×60	5e+04	86	33	83	13
	90×90	1e+05	127	40	127	15
	120×120	2e+05	170	44	167	15
1a	30×30	1e+05	54	16	54	11
	60×60	4e+05	106	21	105	14
	90×90	1e+06	157	24	157	16
	120×120	2e+06	-	26	-	16
1c	30×30	2e+07	78	38	76	16
	60×60	7e+07	150	53	146	17
	90×90	1e+08	-	63	-	18
	120×120	2e+08	-	73	-	21

Using phantom node setup is crucial to allow standard graph-based aggregation!

OC: 1.28-1.40

Null Space for Jump & Tip Enrichments

Prolongation/Restriction should preserve zero-energy modes!

2D elasticity problem has 3 Zero Energy Modes (ZEMs):

$$
\begin{array}{c|c|c|c|}
 & 1 & 2 & 3 \\
\hline
 & & \dots & \\
d_{xI} & 1 & 0 & -y\_I \\
d_{yI} & 0 & 1 & x\_I \\
 & & \dots & \\
\hline
\end{array}
$$

Null space for phantom node approach

- Standard DOFs are treated as usual
- Phantom DOFs are treated like Standard DOFs
- Tip DOFs? Tricky…

Null space for shifted enrichment approach

- Enriched DOFs don’t contribute to rigid body motion
  - Put 0 into their respective rows
- Change of basis transformation only for jump enrichment
  - Transform linear system & nullspace

  → Tip DOFs are ignored during prolongation & restriction

  → Tip DOF smoothing only on finest level (fine scale feature)

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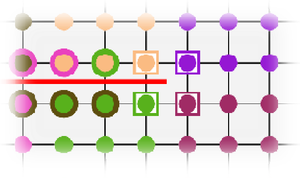
Smoothing

- Finest Level: Use special tip smoother D^{tip} in addition to standard (Block-) Gauss-Seidel smoothing → multiplicative Schwarz



Reason for special smoothing:
- dense blocks (40x40 for quad4)
- high condition number

  - Tip smoother: direct solve for each tip block
  - Pre-smoother

    $$\boldsymbol{u} \leftarrow \mathrm{GaussSeidel}(\boldsymbol{u}, \tilde{\boldsymbol{A}}, \boldsymbol{b})$$

    $$\boldsymbol{u} \leftarrow \boldsymbol{u} + \boldsymbol{D}^{\mathrm{tip}} \cdot (\boldsymbol{b} - \tilde{\boldsymbol{A}} \cdot \boldsymbol{u})$$

  - Post-smoother

    $$\boldsymbol{u} \leftarrow \boldsymbol{u} + \boldsymbol{D}^{\mathrm{tip}} \cdot (\boldsymbol{b} - \tilde{\boldsymbol{A}} \cdot \boldsymbol{u})$$

    $$\boldsymbol{u} \leftarrow \mathrm{GaussSeidel}(\boldsymbol{u}, \tilde{\boldsymbol{A}}, \boldsymbol{b})$$

    Pre-Post-smoother symmetry is important

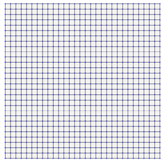
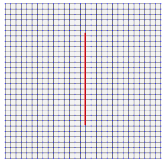
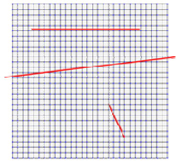
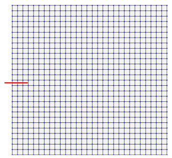
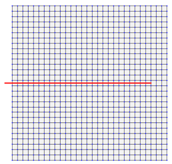
  - 3d geometrical tip-enrichment may require extra splitting of dense blocks

- All coarser levels: standard (Block-) Gauss-Seidel
- Coarsest Level: standard direct solve

Numerical Results for full XFEM system

CG preconditioned with AMG

Special tip smoother is essential to deal with tip enrichments!

Case	$n_e \times n_e$	$\alpha_{\mathrm{cond.}}$	n_{iter}				
			1L	ML	ML, NS	ML, MS	ML, MS, NS
I	30×30	3e+03	32	9	9	9	9
	60×60	1e+04	63	10	10	10	10
	90×90	3e+04	93	11	11	11	11
	120×120	5e+04	123	11	11	11	11
II	30×30	2e+07	115	84	75	21	18
	60×60	8e+08	-	115	97	24	20
	90×90	8e+09	-	141	114	27	23
	120×120	3e+10	-	-	143	28	23
III	30×30	5e+07	143	122	94	24	18
	60×60	1e+09	-	180	158	27	20
	90×90	2e+10	-	-	-	29	20
	120×120	3e+10	-	-	-	37	26
1a	30×30	6e+05	66		31	16	16
	60×60	3e+06	117		31	18	18
	90×90	1e+07	165		33	20	20
	120×120	2e+07	-		32	19	19
1c	30×30	1e+08	86		34	21	20
	60×60	7e+08	157		35	23	23
	90×90	2e+09	-		35	24	24
	120×120	3e+09	-		37	26	26

Operator complexity: 1.28-1.40

Concluding Remarks

Standard SA-AMG methods can be used, if proper input is provided!

Key components:

- System matrix must be in phantom-node form for jump DOF
  - Either you already have it, (voids, fluid-structure interaction, …) , or
  - do a simple transformation $\boldsymbol{G}^{\mathrm{T}} \cdot \boldsymbol{A} \cdot \boldsymbol{G} \cdot \boldsymbol{G}^{-1} \cdot \boldsymbol{u} = \boldsymbol{G}^{\mathrm{T}} \cdot \boldsymbol{f}$
- Simple Null space construction: zero entries for shifted enriched DOF
- Two-step smoothing on finest level (or add your own smoother)

→ Very good convergence behavior.

Current & Future Work

- What happens to tiny element fractions (conditioning)?
- 3d implementation (based on MueLu, the new Multigrid package in Trilinos)

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